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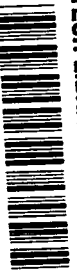


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**THE RUNGE-KUTTA EQUATIONS  
BY QUADRATURE METHODS**

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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

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# THE RUNGE-KUTTA EQUATIONS BY QUADRATURE METHODS

## SUMMARY

This report gives a basically new approach to the formulation of the classic Runge-Kutta process. Dependence on the tedious Taylor expansions is obviated by a matrix equation which defines the Runge-Kutta equations for any order; furthermore, the elements of these matrices are obtained quite simply. The method of quadratures is used to determine the conditions on the parameters which characterize the process since these parameters determine the order of accuracy of these functions.

## INTRODUCTION

We briefly indicate the Runge-Kutta process which leads to an algebraic system of equations whose solutions give the parameters involved.

Consider the initial value problem

$$y' = f(x, y) \quad y(x_0) = y_0. \quad (1)$$

We define the sequence of  $N$  quantities

$$\begin{aligned} k_1 &= hf(x_0, y_0) \\ k_2 &= hf(x_0 + \alpha_2 h, y_0 + \beta_{21} k_1) \\ k_3 &= hf(x_0 + \alpha_3 h, y_0 + \beta_{31} k_1 + \beta_{32} k_2) \\ k_4 &= hf(x_0 + \alpha_4 h, y_0 + \beta_{41} k_1 + \beta_{42} k_2 + \beta_{43} k_3) \\ k_5 &= hf(x_0 + \alpha_5 h, y_0 + \beta_{51} k_1 + \beta_{52} k_2 + \beta_{53} k_3 + \beta_{54} k_4) \end{aligned} \quad (2)$$

⋮  
⋮  
⋮  
⋮

$$k_N = hf(x_0 + \alpha_N h, y_0 + \sum_{j=1}^{N-1} \beta_{Nj} k_j),$$

and the linear form

$$y(x_0 + h) \approx y_0 + \sum_{i=1}^N \omega_i k_i \quad (3)$$

such that the expansion of this in powers of  $h$  agrees with the exact solution of equation (1) to a prescribed number of terms.

It is the usual practice in determining the parameters in equation (2) to expand these functions in Taylor series about the initial point  $(x_0, y_0)$  so that, to a given order, equation (3) is identical with the Taylor expansion

$$y(x_0 + h) = y_0 + hf(x_0, y_0) + \frac{h^2}{2!} f^I(x_0, y_0) + \frac{h^3}{3!} f^{II}(x_0, y_0) + \dots \quad (4)$$

which is the true solution of equation (1). Here the superscripts denote total derivatives with respect to  $x$ , which in terms of the partial derivatives increases in complexity as the order increases. On equating the respective coefficients of the partial derivative in these expansions to a given order in  $h$ , we are led to the system of equations which determine the parameters in equation (2).

When the order of the Runge-Kutta process is reasonably high, the expansions in terms of their respective partial derivatives become somewhat formidable.<sup>1</sup>

With the method we are about to introduce, we shall obviate the need for these tedious Taylor expansions in order to obtain the system of equations which defines the parameters in equation (2); we will have instead a procedure which is almost automatic and extendible to any order.

## THE QUADRATURE METHOD

Consider the quadrature formula<sup>2</sup>

$$\int_a^b f(x) dx \approx \sum_{i=1}^N \omega_i f(x_i) \quad (5)$$

<sup>1</sup> See Kopal's [1] expansion for the fourth-order Runge-Kutta formulation; the magnitude of the task for higher orders becomes evident. The work of Butcher [2-5] and Shanks [6-7] are generalizations based on the approach by Taylor series expansion.

<sup>2</sup> We assume a weight factor of unity in equation (5); obviously the following analysis could be extended to include other weight factors.

which approximates the integral by a linear combination of the values of the function for the arbitrary zeros  $x_i$  ( $i = 1, 2, \dots, N$ ). We say that equation

(5) has the precision  $m$  if it is exact for the successive powers  $f(x) = x^r$  ( $r = 0, 1, \dots, m$ ) (and, therefore, also for all polynomials of degree  $m$ ). This is equivalent to the  $m+1$  equations

$$\int_a^b x^r dx = \sum_{i=1}^N \omega_i x_i^r, \quad r = 0, 1, \dots, m. \quad (6)$$

Suppose now that equation (1) be reformulated as

$$y(x_0 + h) - y(x_0) = \int_{x_0}^{x_0+h} f(x, y(x)) dx \quad (7)$$

in which form it includes the initial conditions. Let us replace the right member of equation (7) by the approximating quadrature sum

$$h \sum_{i=0}^{N-1} \omega_{i+1} f(x_i, y(x_i)) \quad (8)$$

where we have set

$$x_i = x_0 + \alpha_{i+1} h, \quad i = 1, 2, 3, \dots, N-1 \quad (9)$$

$$y_i = y(x_i) = y(x_0 + \alpha_{i+1} h),$$

then for a degree of precision  $m$

$$h(\omega_1 + \omega_2 + \dots + \omega_N) = u_0$$

$$h(\omega_1 x_0 + \omega_2 x_1 + \dots + \omega_N x_{N-1}) = u_1$$

⋮

$$h(\omega_1 x_0^m + \omega_2 x_1^m + \dots + \omega_N x_{N-1}^m) = u_m$$

where, as in equation (6)

$$u_r = \int_{x_0}^{x_0+h} x^r dx = \frac{(x_0+h)^{r+1} - x_0^{r+1}}{r+1}, \quad r = 0, 1, \dots, m. \quad (11)$$

The  $m+1$  linear equations (10), as we shall see, will give us some of the equations in the Runge-Kutta process.

Combining equations (7) and (8),

$$y(x_0 + h) - y(x_0) \approx h \sum_{i=0}^{N-1} \omega_{i+1} f(x_i, y(x_i)) \quad (12)$$

is a quadrature approximation with the degree of precision  $m$  if equation (10) holds.

We continue by making another quadrature approximation, this time for  $y(x_i)$  in equation (12).

For any term  $f(x_i, y_i)$  in (12) we can write

$$y'(x_i) = f(x_i, y_i) = f(x_0 + \alpha_{i+1} h, y(x_0 + \alpha_{i+1} h)) \quad (13)$$

As in equation (7), we can replace equation (13) by the integral form

$$y(x_i) - y_0 = \int_{x_0}^{x_i = x_0 + \alpha_{i+1} h} f(x, y(x)) dx \quad (14)$$

and finally, we can replace the integral by the approximate quadrature sum

$$h \sum_{j=0}^{i-1} \beta_{i+1, j+1} f(x_j, y(x_j))$$

where the  $\beta$ 's correspond to the weight coefficients  $\omega$  in equation (8). For a degree of precision  $m$  equation (10) must be satisfied with the  $\beta$ 's replacing the  $\omega$ 's and  $u_r(\alpha_{i+1})$  replacing  $u_r$  in equation (11) where

$$u_r(\alpha_{i+1}) = \int_{x_0}^{x_0 + \alpha_{i+1} h} x^r dx = \frac{(x_0 + \alpha_{i+1} h)^{r+1} - x_0^{r+1}}{r+1}, \quad r = 0, 1, \dots, m. \quad (15)$$

Summarizing the above, we can replace  $y(x_i)$  in equation (12) with the requisite precision, if we set

$$y(x_i) \approx y_0 + h \sum_{j=0}^{i-1} \beta_{i+1, j+1} f(x_j, y(x_j)) \quad (16)$$

where

$$h(\beta_{i+1, 1} + \beta_{i+1, 2} + \dots + \beta_{i+1, i}) = u_0(\alpha_{i+1})$$

$$\begin{aligned}
& h \left( \beta_{i+1,1} x_0 + \beta_{i+1,2} x_1 + \dots + \beta_{i+1,i} x_{i-1} \right) \\
& = u_1 (\alpha_{i+1}) \\
& \vdots \\
& h \left( \beta_{i+1,1} x_0^m + \beta_{i+1,2} x_1^m + \dots + \beta_{i+1,i} x_{i-1}^m \right) \\
& = u_m (\alpha_{i+1}) \\
& i = 1, 2, \dots, N-1
\end{aligned} \tag{17}$$

must be satisfied to obtain the required precision  $m$ ; where, as we shall see,  $m = p - 1$  with  $p$  the order of the Runge-Kutta process.

By expanding equation (16) consecutively for  $i = 1, 2, \dots$  and by using the approximations for  $y(x_i)$  in each successive expansion, we will finally obtain in place of equation (16)

$$y(x_i) \approx y_0 + \sum_{j=0}^{i-1} \beta_{i+1,j+1} k_{j+1} \quad (18)$$

When this is substituted into equation (12), the functions take the form of the Runge-Kutta expressions defined by equation (2) and the numerical solution equation (3).

## THE RUNGE-KUTTA EQUATIONS

It will be convenient to put some of the previous equations into a more usable form. Thus, for equation (10) we can write

$$h \begin{bmatrix} \omega_1 \omega_2 \dots \omega_N \end{bmatrix} \begin{bmatrix} x_0^j \\ x_1^j \\ \vdots \\ x_{N-1}^j \end{bmatrix} = u_j, \quad j = 0, 1, \dots, m \quad (19)$$

Using (9) and expanding by the binomial theorem, we have

$$\begin{aligned}
x_i^j &= (x_0 + \alpha_{i+1} h)^j \\
&= \begin{bmatrix} 1 & \alpha_{i+1} & \alpha_{i+1}^2 & \dots & \alpha_{i+1}^j \end{bmatrix} \begin{bmatrix} x_0^j \\ j x_0^{j-1} h \\ \vdots \\ h^j \end{bmatrix} \quad (20)
\end{aligned}$$

Similarly, we can put equation (11) in the matrix form

$$u_j = h \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{3} & \dots & \frac{1}{(j+1)} \end{bmatrix} \begin{bmatrix} x_0^j \\ j x_0^{j-1} h \\ \vdots \\ h^j \end{bmatrix} \quad (21)$$

so that we can replace equation (19) by

$$\begin{aligned}
& h \begin{bmatrix} \omega_1 \omega_2 \dots \omega_N \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 1 & \alpha_2 & \alpha_2^2 & \dots & \alpha_2^j \\ 1 & \alpha_3 & \alpha_3^2 & \dots & \alpha_3^j \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \alpha_N & \alpha_N^2 & \dots & \alpha_N^j \end{bmatrix} \begin{bmatrix} x_0^j \\ j x_0^{j-1} h \\ \vdots \\ h^j \end{bmatrix} \\
& = h \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{3} & \dots & \frac{1}{(j+1)} \end{bmatrix} \begin{bmatrix} x_0^j \\ j x_0^{j-1} h \\ \vdots \\ h^j \end{bmatrix} \quad (22)
\end{aligned}$$

$$j = 0, 1, \dots, m$$

If we equate coefficients in equation (22), we get, for any fixed  $j$ , some, and finally (for  $j = m$ ), all of the equations

$$\begin{aligned}
& \begin{bmatrix} \omega_1 \omega_2 \dots \omega_N \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 1 & \alpha_2 & \alpha_2^2 & \dots & \alpha_2^m \\ 1 & \alpha_3 & \alpha_3^2 & \dots & \alpha_3^m \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \alpha_N & \alpha_N^2 & \dots & \alpha_N^m \end{bmatrix} \\
& = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{3} & \dots & \frac{1}{(m+1)} \end{bmatrix} \quad (23)
\end{aligned}$$

which replace equation (10) and which constitute a part of the Runge-Kutta equations.<sup>3</sup>

We can treat equation (17) similarly and write

$$h \begin{bmatrix} \beta_{i+1,1} & \beta_{i+1,2} & \dots & \beta_{i+1,i} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 1 & \alpha_2 & \alpha_2^2 & \dots & \alpha_2^j \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \alpha_i & \alpha_i^2 & \dots & \alpha_i^j \end{bmatrix} \begin{bmatrix} x_0^j \\ j x_0^{j-1} h \\ \vdots \\ h^j \end{bmatrix} = u_j(\alpha_{i+1}) \quad \begin{matrix} i = 1, 2, \dots, (N-1) \\ j = 0, 1, \dots, m \end{matrix} \quad (24)$$

and as in (21) for  $u_j$ , we can write for equation (15)

$$u_j(\alpha_{i+1}) = h \begin{bmatrix} \alpha_{i+1} & \frac{1}{2} \alpha_{i+1}^2 & \frac{1}{3} \alpha_{i+1}^3 & \dots & \frac{1}{(j+1)} \alpha_{i+1}^{j+1} \end{bmatrix} \begin{bmatrix} x_0^j \\ j x_0^{j-1} h \\ \vdots \\ h^j \end{bmatrix} \quad j = 0, 1, \dots, m. \quad (25)$$

Substituting this into equation (24) and equating coefficients for all fixed  $j$ 's, we can summarize our result by replacing equation (17) with

$$\begin{bmatrix} \beta_{i+1,2} & \dots & \beta_{i+1,i} \end{bmatrix} \begin{bmatrix} \alpha_2 & \alpha_2^2 & \dots & \alpha_2^j \\ \alpha_3 & \alpha_3^2 & \dots & \alpha_3^j \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_i & \alpha_i^2 & \dots & \alpha_i^j \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \alpha_{i+1}^2 & \dots & \frac{1}{(j+1)} \alpha_{i+1}^{j+1} \end{bmatrix} \quad \begin{matrix} i = 2, 3, \dots, (N-1) \\ j = 1, 2, \dots, m \end{matrix} \quad (26)$$

and

$$\alpha_{i+1} = \beta_{i+1,1} + \beta_{i+1,2} + \dots + \beta_{i+1,i}, \quad i = 1, 2, \dots, (N-1), \quad (27)$$

<sup>3</sup>For the solution of equation (23), with  $\omega_i$  in terms of the  $\alpha$ 's, see [8] and [9].

the latter being the first equation in equations (17). The equations (27) are always assumed in the Runge-Kutta process as basic relations between the parameters in equations (2).

We might also require that the equations

$$\beta_{i+1,2} \alpha_2 + \beta_{i+1,3} \alpha_3 + \dots + \beta_{i+1,i} \alpha_i = \frac{1}{2} \alpha_{i+1}^2 \quad i = 2, 3, \dots, N-1 \quad (28)$$

hold. These and similar equations obtained from equation (26), however, are not specifically assumed here when deriving the Runge-Kutta equations but are sometimes invoked in reducing the number of Runge-Kutta equations (for  $p > 4$ ) when solving for the parameters.

We now come to an important step in deriving the classical Runge-Kutta equations. We form the following weighted expressions using equations (17) (but excluding the first equation, or equations (27)):

$$\sum_{i=1}^{N-1} \omega_{i+1} u_j(\alpha_{i+1}), \quad j = 1, 2, \dots, m \quad (29)$$

or, using equations (26)

$$\Omega_{3,N}^1 \begin{bmatrix} \beta_{32} & 0 & \dots & 0 \\ \beta_{42} & \beta_{43} & \dots & \beta_{4,N-1} \\ \vdots & \vdots & \ddots & \vdots \\ \beta_{N2} & \beta_{N3} & \dots & \beta_{N,N-1} \end{bmatrix} \begin{bmatrix} \alpha_2 & \alpha_2^2 & \dots & \alpha_2^m \\ \alpha_3 & \alpha_3^2 & \dots & \alpha_3^m \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{N-1} & \alpha_{N-1}^2 & \dots & \alpha_{N-1}^m \end{bmatrix} = \Omega_{2,N}^1 \begin{bmatrix} \frac{1}{2} \alpha_2^2 & \dots & \frac{1}{(m+1)} \alpha_2^{m+1} \\ \frac{1}{2} \alpha_3^2 & \dots & \frac{1}{(m+1)} \alpha_3^{m+1} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{2} \alpha_N^2 & \dots & \frac{1}{(m+1)} \alpha_N^{m+1} \end{bmatrix} \quad (30)$$

where

$$\Omega_{2,N}^1 = (\omega_2 \omega_3 \dots \omega_N) \quad \Omega_{3,N}^1 = (\omega_3 \omega_4 \dots \omega_N) \quad (31)$$



If we now set

$$\begin{aligned} c_3^{(j)} &= \beta_{32} \alpha_2^j \\ c_4^{(j)} &= \beta_{42} \alpha_2^j + \beta_{43} \alpha_3^j \\ &\vdots \\ c_N^{(j)} &= \beta_{N2} \alpha_2^j + \beta_{N3} \alpha_3^j + \dots + \beta_{N,N-1} \alpha_{N-1}^j \end{aligned}$$

$j = 1, 2, \dots, m-1$

(32)

then matrix equation (30) becomes

$$\Omega_{3,N}^1 \begin{bmatrix} c_3^{(1)} & c_3^{(2)} & \dots & c_3^{(m-1)} \\ c_4^{(1)} & c_4^{(2)} & \dots & c_4^{(m-1)} \\ \vdots & \vdots & \ddots & \vdots \\ c_N^{(1)} & c_N^{(2)} & \dots & c_N^{(m-1)} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \left( \frac{1}{3} \right) & \frac{1}{3} \left( \frac{1}{4} \right) & \dots & \frac{1}{m-1} \left( \frac{1}{m} \right) \\ \frac{1}{2} \left( \frac{1}{4} \right) & \frac{1}{3} \left( \frac{1}{5} \right) & \dots & \frac{1}{m-1} \left( \frac{1}{m+1} \right) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{2} \left( \frac{1}{m+1} \right) & \dots & \dots & \dots \end{bmatrix} \quad (33)$$

where we have used equation (23) to evaluate the matrix product in the right member of equation (30) except in the last column where it was not possible and which we have suppressed in both sides of (33) since they yield higher order terms and are not relevant to our degree of precision.

Equation (33) gives us another set of Runge-Kutta equations. If we return to equations (29) and the subsequent analysis, it should be apparent that we should be able to find other relevant Runge-Kutta equations if we replaced  $\omega_{i+1}$  in (29) by  $\omega_{i+1} \alpha_{i+1}^n$  with  $n = 1, 2, \dots, m-2$ .

Therefore, if we write

$$\begin{aligned} \Omega_{2,N}^{(m-1)} &= \begin{bmatrix} \omega_2 & \dots & \omega_N \\ \omega_2 \alpha_2 & \dots & \omega_N \alpha_N \\ \vdots & \ddots & \vdots \\ \omega_2 \alpha_2^{m-2} & \dots & \omega_N \alpha_N^{m-2} \end{bmatrix} \\ \Omega_{3,N}^{(m-1)} &= \begin{bmatrix} \omega_3 & \dots & \omega_N \\ \omega_3 \alpha_3 & \dots & \omega_N \alpha_N \\ \vdots & \ddots & \vdots \\ \omega_3 \alpha_3^{m-2} & \dots & \omega_N \alpha_N^{m-2} \end{bmatrix} \end{aligned} \quad (34)$$

we should be able to replace the row vectors  $\Omega_{3,N}^1$  and  $\Omega_{2,N}^1$  in equation (30) by the  $(m-1)$ -rowed matrices in equation (34). This gives

$$\Omega_{3,N}^{(m-1)} C = \begin{bmatrix} \frac{1}{2} \left( \frac{1}{3} \right) & \frac{1}{3} \left( \frac{1}{4} \right) & \dots & \frac{1}{m-1} \left( \frac{1}{m} \right) & \frac{1}{m} \left( \frac{1}{m+1} \right) \\ \frac{1}{2} \left( \frac{1}{4} \right) & \frac{1}{3} \left( \frac{1}{5} \right) & \dots & \frac{1}{m-1} \left( \frac{1}{m+1} \right) & \dots \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{1}{2} \left( \frac{1}{m+1} \right) & \dots & \dots & \dots & \dots \end{bmatrix} \quad (35)$$

where the substitution of C for the matrix in equation (33) is evident. Thus, we have extended the number of Runge-Kutta equations by equation (35); but others, as we shall see, are possible. It might be appropriate to refer to the elements of  $\Omega_{3,N}^{(m-1)}$  and other similar elements which we will form as generalized Runge-Kutta weights.

It should be apparent that if we could find all the other pertinent sets of generalized Runge-Kutta weights, we should be able to find all the relevant Runge-Kutta equations. The procedure for doing this is reasonably simple. As we obtain new Runge-Kutta equations we must examine each for new generalized Runge-Kutta weights which in turn may generate new equations. The simplest way to recognize these are as the coefficients of  $\alpha_i^n$ , for appropriate integral values of n, of the already known Runge-Kutta equations. The two specific examples -- for orders four and five -- which will be given should sufficiently illustrate the procedure.

We might finally summarize our results. The Runge-Kutta equations for N evaluations in equations (2), with N appropriately chosen, and order  $p=m-1$  are given by equations (23), (27), (35) and all additional Runge-Kutta generalized weight coefficients that can be found to replace  $\Omega_{3,N}^1$  in equation (30). This will result in an appropriate extension of equation (35), wherein the matrix which contains all the Runge-Kutta weight coefficients will, for convenience, be referred to as  $\Omega$ .

It might be noted that we also use equation (28). Then, because of equations (32),  $c_{i+1}^{(1)} = \frac{1}{2} \alpha_{i+1}^2$  ( $i = 2, 3, \dots, (N-1)$ ); and, as may be seen from equation (33), the number of Runge-Kutta equations is reduced.

## FOURTH-ORDER RUNGE-KUTTA EQUATIONS

We will illustrate the preceding work, using our quadrature method, for the particular fourth-order Runge-Kutta process and show how to derive the equations which define the parameters  $\alpha_i$  and

$$\beta_{ij}^*$$

We first replace the right member of equation (7) by a quadrature sum involving the four<sup>4</sup> arbitrary zeros  $x_i$  ( $i = 0, 1, 2, 3$ ), so that corresponding to equation (12), we have

$$y(x_0 + h) - y(x_0) \approx h [\omega_1 f(x_0, y_0) + \omega_2 f(x_1, y_1) + \omega_3 f(x_2, y_2) + \omega_4 f(x_3, y_3)] \quad (36)$$

where  $x_i$  and  $y_i$  are defined by equation (9). We will require a degree of precision of three, not four, in equations (10) because of the factor  $h$  in (36).

We will now replace the  $y_i$  ( $i = 1, 2, 3$ ) in (36) to the degree of precision three in accordance with the analysis previously given. Thus, the first term in equation (36) which will be affected by quadratures for  $y(x_i)$  is  $f(x_1, y_1)$ , which is to be replaced by

$$f(x_0 + \alpha_2 h, y_0 + \beta_{21} k_1) \quad (37)$$

as may be seen from equations (2). By equation (14)

$$y(x_1) - y_0 = \int_{x_0}^{x_0 + \alpha_2 h} f(x, y(x)) dx \quad (38)$$

and after approximating the integral with the quadrature equation (16), and using  $k_1$  defined in equations (2),

$$y_1 - y_0 = (h \beta_{21}) f(x_0, y_0) = \beta_{21} k_1 \quad (39)$$

where, according to equations (17), the weight coefficient  $(h \beta_{21})$  must satisfy the following four conditions if the quadrature is to have a degree of precision three

<sup>4</sup> We are anticipating the fact that for the fourth-order process only four arbitrary zeros are necessary. This equality between the order and the number of function evaluations,  $N$ , only holds for orders up to the fourth. For higher orders this relation is complex; Butcher [5] deals with this problem.

$$(h \beta_{21}) x_0^r = u_r(\alpha_2), \quad r = 0, 1, 2, 3 \quad (40)$$

where  $u_r(\alpha_2)$  is given by equation (15).

In similar fashion we replace  $y_2$  and  $y_3$  in equation (36) by making the respective quadratures indicated by equation (16)

$$y_2 - y_0 = (h \beta_{31}) f(x_0, y_0) + (h \beta_{32}) f(x_1, y_1) \quad (41)$$

$$y_3 - y_0 = (h \beta_{41}) f(x_0, y_0) + (h \beta_{42}) f(x_1, y_1) + (h \beta_{43}) f(x_2, y_2) \quad (42)$$

where  $(h \beta_{ij})$  may again be interpreted as the weight coefficients in the quadratures.

Equation (39), which defines  $y_1$  with the requisite precision, can be used to replace  $y_1$  in equation (41). Then

$$y_2 - y_0 \approx \beta_{31} h f(x_0, y_0) + \beta_{32} h f(x_1, y_0 + \beta_{21} k_1)$$

so that, with  $k_1$  and  $k_2$  defined as in equations (2),

$$y_2 \approx y_0 + \beta_{31} k_1 + \beta_{32} k_2 \quad (43)$$

In a similar fashion, by using both equations (39) and (43), we can replace equation (42) with

$$y_3 \approx y_0 + \beta_{41} k_1 + \beta_{42} k_2 + \beta_{43} k_3 \quad (44)$$

where the  $k$ 's are defined by equations (2). This procedure, as will be observed, replaces  $y_i$  in  $f(x_i, y_i)$  with the same degree of precision as the degree of precision in the quadrature (36).

Again, in order that the required degree of precision be at least of order three, the weights in equations (41) and (42) must according to (17) satisfy, respectively, the equations

$$(h \beta_{31}) x_0^r + (h \beta_{32}) x_1^r = u_r(\alpha_3), \quad r = 0, 1, 2, 3 \quad (45)$$

and

$$(h \beta_{41}) x_0^r + (h \beta_{42}) x_1^r + (h \beta_{43}) x_2^r = u_r(\alpha_4), \quad r = 0, 1, 2, 3 \quad (46)$$

where  $u_r(\alpha_3)$  and  $u_r(\alpha_4)$  are given by equation (15) and  $x_i$  by equations (9).

Our problem is to satisfy the conditions (40), (45), and (46), so that the repeated quadratures we have made represent the Runge-Kutta process to the necessary degree of precision. Rather than use the general results we have derived, we will illustrate our procedure in some detail.

## CONDITIONS FOR A FOURTH-ORDER RUNGE-KUTTA PROCESS

We have seen that in order that the degree of precision represented by the bracketed term in equation (36) be at least of order three in  $h$ , the four conditions given by equations (10) must hold. If we replace  $x_i$  by equation (9) and  $u_i$  by equation (11), equations (10) gives

$$\begin{aligned}\omega_1 + \omega_2 + \omega_3 + \omega_4 &= 1 \\ \omega_2 \alpha_2 + \omega_3 \alpha_3 + \omega_4 \alpha_4 &= \frac{1}{2} \\ \omega_2 \alpha_2^2 + \omega_3 \alpha_3^2 + \omega_4 \alpha_4^2 &= \frac{1}{3} \\ \omega_2 \alpha_2^3 + \omega_3 \alpha_3^3 + \omega_4 \alpha_4^3 &= \frac{1}{4}\end{aligned}\quad (47)$$

which may have been anticipated by using equation (23) with  $m = 3$ .

Four more equations are necessary for the Runge-Kutta process which we will now derive, but which for convenience we anticipate here. These are:

$$(\omega_3 \beta_{32} + \omega_4 \beta_{42}) \alpha_2 + (\omega_4 \beta_{43}) \alpha_3 = \frac{1}{6} \quad (48)$$

$$(\omega_3 \beta_{32} + \omega_4 \beta_{42}) \alpha_2^2 + (\omega_4 \beta_{43}) \alpha_3^2 = \frac{1}{12} \quad (49)$$

$$(\omega_3 \alpha_3) (\beta_{32} \alpha_2) + (\omega_4 \alpha_4) + (\beta_{42} \alpha_2 + \beta_{43} \alpha_3) = \frac{1}{8} \quad (50)$$

$$(\omega_4 \beta_{43}) \beta_{32} \alpha_2 = \frac{1}{24} \quad (51)$$

We now return to the conditions (40), (45) and (46), which we shall satisfy in the following manner. The equations arising from  $u_0(\alpha_i)$  ( $i = 2, 3, 4$ ) can be satisfied identically by using equation (15), so that

$$\begin{aligned}\alpha_2 &= \beta_{21} \\ \alpha_3 &= \beta_{31} + \beta_{32} \\ \alpha_4 &= \beta_{41} + \beta_{42} + \beta_{43} \quad (52)\end{aligned}$$

These are additional relations which hold for the fourth-order Runge-Kutta process and may have been found directly from equations (27).

Let us now consider the expressions formed by

$$\omega_2 u_1(\alpha_2) + \omega_3 u_1(\alpha_3) + \omega_4 u_1(\alpha_4), \quad i = 1, 2, 3. \quad (53)$$

As an example, when  $i = 2$ , this will give, if we use equation (15),

$$\begin{aligned}(x_0^2 h) [\omega_2 \alpha_2 + \omega_3 \alpha_3 + \omega_4 \alpha_4] \\ + x_0 h^2 [\omega_2 \alpha_2^2 + \omega_3 \alpha_3^2 + \omega_4 \alpha_4^2] \\ + 1/3 h^3 [\omega_2 \alpha_2^3 + \omega_3 \alpha_3^3 + \omega_4 \alpha_4^3]\end{aligned}\quad (54)$$

and by equations [47] this becomes

$$\frac{1}{2} (x_0^2 h) + \frac{1}{3} x_0 h^2 + \frac{1}{4} \left( \frac{1}{3} h^3 \right) \quad (55)$$

which is free from the weights  $\omega_i$  and parameters  $\alpha_i$  and  $\beta_{ij}$ .

The corresponding expression for equations (53), if we use equations (40), (45) and (46), is

$$\begin{aligned}x_0^2 h [\omega_2 \alpha_2 + \omega_3 \alpha_3 + \omega_4 \alpha_4] \\ + 2 x_0 h^2 [(\omega_3 \beta_{32} + \omega_4 \beta_{42}) \alpha_2 + (\omega_4 \beta_{43}) \alpha_3] \\ + h^3 [(\omega_3 \beta_{32} + \omega_4 \beta_{42}) \alpha_2^2 + (\omega_4 \beta_{43}) \alpha_3^2]\end{aligned}\quad (56)$$

so that if we equate the coefficients of equations (55) and (56), we obtain three equations for the fourth-order Runge-Kutta formulation -- equations (48) and (49), and one which is a repetition of an equation in equations (47). No new results will be derived if we treat similarly (53) when  $i = 1, 3$ .

It will be observed that if we replace  $\omega_i$  in equations (53) by  $\omega_i \alpha_i$ , the resulting expression corresponding to equation (55) will again contain terms which are free of parameters; in fact, we are led to the new equation (50). This is an extension of the process we have described and which leads to the concept of the generalized Runge-Kutta weight coefficients; and, as we have pointed out, if we can find all sets of these coefficients which are relevant to a particular order of the Runge-Kutta process, we will produce all the Runge-Kutta equations. We continue with our coefficients by seeking contributions to these from each new equation as it is generated. These are, in our present case, the coefficients of  $\alpha_i$  and  $\alpha_i^2$  in equations (48) and (49) which contribute a new set of

generalized Runge-Kutta weight coefficients which generate the new equation (51)<sup>5</sup>.

We can summarize these results by the extension of the matrix equation (35) which was derived by a generalization of the elementary concepts presented here for the fourth-order case. This gives

$$\begin{bmatrix} \omega_3 & \omega_4 \\ \omega_3 \alpha_3 & \omega_4 \alpha_4 \\ \omega_4 \beta_{43} & 0 \end{bmatrix} \begin{bmatrix} \beta_{32} \alpha_2 & \beta_{32} \alpha_2^2 \\ (\beta_{42} \alpha_2 + \beta_{43} \alpha_3) (\beta_{42} \alpha_2^2 + \beta_{43} \alpha_3^2) \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \left( \frac{1}{3} \right) & \frac{1}{3} \left( \frac{1}{4} \right) \\ \frac{1}{2} \left( \frac{1}{4} \right) & \text{---} \\ \frac{1}{2} \left( \frac{1}{12} \right) & \text{---} \end{bmatrix} \quad (57)$$

which represents the results given by equations (48) through (51).

## THE FIFTH-ORDER RUNGE-KUTTA EQUATIONS

Several aspects on formulating the matrix  $\Omega$ , which contains all the generalized Runge-Kutta weight coefficients, can best be illustrated by considering the fifth-order case, which required at least six evaluations for a solution [4, 6].

We start with the applicable Runge-Kutta equations given by equations (23) and (27) with  $N = 6$  and  $m = 4$ . We then enumerate the generalized Runge-Kutta weight coefficients; starting initially with the three rows given by equations (34) and followed by the subsequent extensions as new Runge-Kutta equations are derived. This gives

$$\Omega = \begin{bmatrix} \omega_3 & \omega_4 & \omega_5 & \omega_6 \\ \omega_3 \alpha_3 & \omega_4 \alpha_4 & \omega_5 \alpha_5 & \omega_6 \alpha_6 \\ \omega_3 \alpha_3^2 & \omega_4 \alpha_4^2 & \omega_5 \alpha_5^2 & \omega_6 \alpha_6^2 \\ \gamma_3^{(0)} & \gamma_4^{(0)} & \gamma_5^{(0)} & 0 \\ \gamma_3^{(1)} \alpha_3 & \gamma_4^{(1)} \alpha_4 & \gamma_5^{(1)} \alpha_5 & 0 \\ \gamma_3^{(1)} & \gamma_4^{(1)} & \gamma_5^{(1)} & 0 \\ \omega_3 c_3^{(1)} & \omega_4 c_4^{(1)} & \omega_5 c_5^{(1)} & \omega_6 c_6^{(1)} \\ (\gamma_4^{(0)} \beta_{43} + \gamma_5^{(0)} \beta_{53}) & \gamma_5^{(0)} \beta_{54} & 0 & 0 \end{bmatrix} \quad (58)$$

<sup>5</sup> Other generalized Runge-Kutta weight coefficients which may be obtained from equations (48) through (51) may be ignored, if we keep in mind that in the Runge-Kutta equations we seek no term which is a product of the  $\alpha$ 's and  $\beta$ 's may have the sum of its powers exceed  $m = p - 1$ .

where the  $c_i^{(1)}$  ( $i = 3, 4, 5, 6$ ) are defined by equations (32) and where the new quantities introduced are given by

$$\begin{bmatrix} \omega_3 \alpha_3^n & \omega_4 \alpha_4^n & \dots & \omega_N \alpha_N^n \end{bmatrix} \begin{bmatrix} \beta_{32} & 0 & \dots & 0 \\ \beta_{42} & \beta_{43} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \beta_{N2} & \beta_{N3} & \dots & \beta_{N,N-1} & 0 \end{bmatrix} = \begin{bmatrix} \gamma_2^{(n)} & \gamma_3^{(n)} & \dots & \gamma_N^{(n)} \end{bmatrix}, \quad n = 0, 1, \dots \quad (59)$$

The Runge-Kutta equations for the fifth order will then be given by extending equation (35):

$$\Omega C = \begin{bmatrix} \frac{1}{2} \left( \frac{1}{3} \right) & \frac{1}{3} \left( \frac{1}{4} \right) & \frac{1}{4} \left( \frac{1}{5} \right) \\ \frac{1}{2} \left( \frac{1}{4} \right) & \frac{1}{3} \left( \frac{1}{5} \right) & \text{---} \\ \frac{1}{2} \left( \frac{1}{5} \right) & \text{---} & \text{---} \\ \frac{1}{2} \left[ \frac{1}{3} \left( \frac{1}{4} \right) \right] & \frac{1}{3} \left[ \frac{1}{4} \left( \frac{1}{5} \right) \right] & \text{---} \\ \frac{1}{2} \left[ \frac{1}{4} \left( \frac{1}{5} \right) \right]^* & \text{---} & \text{---} \\ \frac{1}{2} \left[ \frac{1}{3} \left( \frac{1}{5} \right) \right]^* & \text{---} & \text{---} \\ \frac{1}{2} \left[ \frac{1}{2} \left( \frac{1}{5} \right) \right] & \text{---} & \text{---} \\ \frac{1}{2} \left[ \frac{1}{3} \left( \frac{1}{4} \right) \left( \frac{1}{5} \right) \right] & \text{---} & \text{---} \end{bmatrix} \quad (60)$$

where  $C$  is a  $(4 \times 3)$  matrix defined in equation (33), and where the numerical values of the elements in the right hand matrix in equation (60) may be readily verified partly by equation (23) and partly by equation (30);<sup>6</sup> and the other by using the new Runge-Kutta equations for the fifth order as they are generated. The dashes in this matrix indicate that there are no results relevant to our problem.<sup>7</sup>

If two of these equations (those obtained from the fifth and sixth row of  $\Omega$  in equation (58) and marked with asterisks in equation (60)) are added, instead

<sup>6</sup> The first three rows may be directly obtained from equation (35).

<sup>7</sup> Except, perhaps, for higher order terms which may be of interest in evaluating error terms.

of being satisfied simultaneously, we get the set of Runge-Kutta equations for the fifth order customarily given in the literature.<sup>8</sup>

## THE GENERALIZED RUNGE-KUTTA WEIGHT MATRIX

We shall now indicate a device whereby we can generate the matrix of equation [58] quite easily. The convenience of this device would be realized if we attempted to generate  $\Omega$  from the basic definition of the generalized Runge-Kutta weights previously given. Even for the relatively simple case of the fifth order the latter process is extremely tedious; furthermore, the evaluation of the numerical matrix [60] is laborious and there is, additionally, the possibility of overlooking some rows of  $\Omega$  if the order is high.

The procedure we will now introduce is quite simple and we will illustrate it for equation (58). We start with the first three rows as required by equations (34) with  $m = 4$ . We next replace  $\omega_i$  ( $i = 3, 4, 5, 6$ ) consecutively by its corresponding terms  $\gamma_i^{(0)}, \gamma_i^{(1)}, \gamma_i^{(2)}, \dots$  ( $i = 3, 4, 5, 6$ ) where the latter terms are defined by (59). This contributes the fourth and sixth rows to the  $\Omega$ -matrix as we reject  $\gamma_i^{(2)}, \gamma_i^{(3)}, \dots$  since the total degree of these terms (the sum of the exponents of the  $\alpha$ 's and  $\beta$ 's) would be too high.<sup>9</sup> We now repeat this procedure replacing  $\omega_i$ , as before, in the  $\omega_i \alpha_i$  and  $\omega_i \alpha_i^2$  rows of equation (58) -- retaining only those terms within the limitations imposed on the total degree of the resulting elements. Thus, we reject  $\gamma_i^{(0)} \alpha_i^2$  whose total degree is three and retain only the elements  $\gamma_i^{(0)} \alpha_i$  in the fifth row.

We continue to make analogous substitutions in the elements of the new rows generated. Let us write  $\gamma_i^{(0)} (\omega_i)$  for  $\gamma_i^{(0)}$  to show, as we may see by equation (59), that  $\gamma_i^{(0)}$  explicitly involves  $\omega_i$  (the same is true for  $\gamma_i^{(1)}, \gamma_i^{(2)}, \dots$  though we will not

<sup>8</sup> The Runge-Kutta equations obtained here may be checked with the equations given by Luther and Konen [10] who use a slightly different notation.

<sup>9</sup> The total degree (see footnote 5) of the fifth-order generalized Runge-Kutta weight coefficients in equations (58) cannot exceed  $m - 2$ . This is because its products with  $c_i^{(1)}$  (whose total degree is two) will give the maximum total degree permissible for the fifth-order case.

need these in this case); and let us replace  $\omega_i$ , as

we did before, by  $\gamma_i^{(0)}, \gamma_i^{(1)}, \dots$  and designate these by  $\gamma_i^{(0)} \left( \gamma_j^{(0)} \right), \gamma_i^{(0)} \left( \gamma_j^{(1)} \right), \dots$ , so that for example

$$\gamma_3^{(0)} \left( \gamma_j^{(0)} \right) = \gamma_4^{(0)} \beta_{43} + \gamma_5^{(0)} \beta_{53} + \gamma_6^{(0)} \beta_{63}$$

$$\gamma_3^{(1)} \left( \gamma_j^{(0)} \right) = \gamma_4^{(0)} \beta_{43} \alpha_4 + \gamma_5^{(0)} \beta_{53} \alpha_5 + \gamma_6^{(0)} \beta_{63} \alpha_6$$

where  $\gamma_6^{(0)} = 0$  in the present case. These again, as

we will show, are generalized Runge-Kutta weight coefficients. In this case, after rejecting those elements whose degrees are too high, we retain only

$\gamma_i^{(0)} \left( \gamma_j^{(0)} \right)$  the elements of the eighth row in (58).

One further addition to our catalogue of terms must be made. We should, generally, add to our matrix such rows as  $\omega_i c_i^{(1)} \alpha_i^n, \omega_i c_i^{(2)} \alpha_i^n \dots$  ( $i = 3, 4, \dots, N; n = 0, 1, \dots, (m - 4)$ ). In our specific case only  $\omega_i c_i^{(1)}$  (the seventh row in equation (58)) is tenable. These elements, too, may be subjected to the substitutions indicated above to give us terms like  $\gamma_i^{(0)} c_i^{(1)}, \gamma_i^{(0)} c_i^{(1)} \alpha_i$ , etc.

We will now justify the rules we have just given for constructing the  $\Omega$ -matrix and show that the entities we obtain are generalized Runge-Kutta weights. Since the generalization to any order would be obvious in what follows, we will, for the sake of brevity, continue with the demonstration for the fifth-order case with six evaluations.

Using equation (30), we can write

$$\begin{bmatrix} \omega_3 & \dots & \omega_6 \\ \omega_3 \alpha_3 & \dots & \omega_6 \alpha_6 \\ \omega_3 \alpha_3^2 & \dots & \omega_6 \alpha_6^2 \end{bmatrix} \begin{bmatrix} \beta_{32} & 0 & 0 & 0 \\ \beta_{42} & \beta_{43} & 0 & 0 \\ \beta_{52} & \beta_{53} & \beta_{54} & 0 \\ \beta_{62} & \beta_{63} & \beta_{64} & \beta_{65} \end{bmatrix} \begin{bmatrix} \alpha_2 \alpha_2^2 \alpha_2^3 \\ \alpha_3 \alpha_3^2 \alpha_3^3 \\ \alpha_4 \alpha_4^2 \alpha_4^3 \\ \alpha_5 \alpha_5^2 \alpha_5^3 \end{bmatrix} \\ = \begin{bmatrix} \omega_2 \omega_3 & \dots & \omega_6 \\ \omega_2 \alpha_2 \omega_3 \alpha_3 & \dots & \omega_6 \alpha_6 \\ \omega_2 \alpha_2^2 \omega_3 \alpha_3^2 & \dots & \omega_6 \alpha_6^2 \end{bmatrix} \begin{bmatrix} \frac{1}{2} \alpha_2^2 & \frac{1}{3} \alpha_2^3 & \frac{1}{4} \alpha_2^4 \\ \frac{1}{2} \alpha_3^2 & \frac{1}{3} \alpha_3^3 & \frac{1}{4} \alpha_3^4 \\ \vdots & \vdots & \vdots \\ \frac{1}{2} \alpha_6^2 & \frac{1}{3} \alpha_6^3 & \frac{1}{4} \alpha_6^4 \end{bmatrix} \quad (61)$$

and using equation (59) on the left side, we get

$$\begin{aligned}
& \begin{bmatrix} \gamma_2^{(0)} & \gamma_3^{(0)} & \gamma_4^{(0)} & \gamma_5^{(0)} \\ \gamma_2^{(1)} & \gamma_3^{(1)} & \gamma_4^{(1)} & \gamma_5^{(1)} \\ \gamma_2^{(2)} & \gamma_3^{(2)} & \gamma_4^{(2)} & \gamma_5^{(2)} \end{bmatrix} \begin{bmatrix} \alpha_2 & \alpha_2^2 & \alpha_2^3 \\ \vdots & \vdots & \vdots \\ \alpha_5 & \alpha_5^2 & \alpha_5^3 \end{bmatrix} \\
&= \begin{bmatrix} \frac{1}{2} \left( \frac{1}{3} \right) & \frac{1}{3} \left( \frac{1}{4} \right) & \frac{1}{4} \left( \frac{1}{5} \right) \\ \frac{1}{2} \left( \frac{1}{4} \right) & \frac{1}{3} \left( \frac{1}{5} \right) & \text{---} \\ \frac{1}{2} \left( \frac{1}{5} \right) & \text{---} & \text{---} \end{bmatrix} \quad (62)
\end{aligned}$$

where the right member of equation (61) has been evaluated by equation (23). From equation (62) it may be seen that since the terms  $\gamma_i^{(n)} \alpha_i^j$  ( $n=0, 1, 2$ ;  $j=0, 1, 2, 3$ ) are coefficients of  $\alpha^q$  in Runge-Kutta equations, they fulfill the basic definition of generalized Runge-Kutta weight coefficients.<sup>10</sup>

If now in equation (61) we replace  $\omega_i$  by  $\gamma_i^{(0)}$  we get<sup>11</sup>

$$\begin{aligned}
& \begin{bmatrix} \gamma_2^{(0)} \left( \gamma_i^{(0)} \right) \dots \gamma_5^{(0)} \left( \gamma_i^{(0)} \right) \\ \gamma_2^{(1)} \left( \gamma_i^{(0)} \right) \dots \gamma_5^{(1)} \left( \gamma_i^{(0)} \right) \\ \gamma_2^{(2)} \left( \gamma_i^{(0)} \right) \dots \gamma_5^{(2)} \left( \gamma_i^{(0)} \right) \end{bmatrix} \begin{bmatrix} \alpha_2 & \alpha_2^2 & \alpha_2^3 \\ \alpha_3 & \alpha_3^2 & \alpha_3^3 \\ \alpha_4 & \alpha_4^2 & \alpha_4^3 \\ \alpha_5 & \alpha_5^2 & \alpha_5^3 \end{bmatrix} \\
&= \begin{bmatrix} \gamma_2^{(0)} & \gamma_3^{(0)} & \dots & \gamma_6^{(0)} \\ \gamma_2^{(0)} \alpha_2 & \gamma_3^{(0)} \alpha_3 & \dots & \gamma_6^{(0)} \alpha_6 \\ \gamma_2^{(0)} \alpha_2^2 & \gamma_3^{(0)} \alpha_3^2 & \dots & \gamma_6^{(0)} \alpha_6^2 \end{bmatrix} \begin{bmatrix} \frac{1}{2} \alpha_2^2 & \frac{1}{3} \alpha_3^3 & \frac{1}{4} \alpha_4^4 \\ \vdots & \vdots & \vdots \\ \frac{1}{2} \alpha_6^2 & \frac{1}{3} \alpha_6^3 & \frac{1}{4} \alpha_6^4 \end{bmatrix} \\
&= \begin{bmatrix} \frac{1}{2} \left( \frac{1}{3} \frac{1}{4} \right) & \frac{1}{3} \left( \frac{1}{4} \frac{1}{5} \right) & \frac{1}{4} \left( \frac{1}{5} \frac{1}{6} \right) \\ \frac{1}{2} \left( \frac{1}{4} \frac{1}{5} \right) & \frac{1}{3} \left( \frac{1}{5} \frac{1}{6} \right) & \text{---} \\ \frac{1}{2} \left( \frac{1}{5} \frac{1}{6} \right) & \text{---} & \text{---} \end{bmatrix} \quad (63)
\end{aligned}$$

where the last matrix product was evaluated by using equation (62). Thus, we have demonstrated that entities of the type  $\gamma_i^{(n)} \left( \gamma_j^{(0)} \right) \alpha_i^m$  (where  $m$  may be 0) are also generalized Runge-Kutta weight coefficients. These simpler cases may be compounded

<sup>10</sup> Note from equations (59) that the missing  $\gamma_6^{(n)}$  ( $n=0, 1, 2$ ) in (62) are zero.

<sup>11</sup>  $\gamma_5^{(0)} \left[ \gamma_i^{(0)} \right] = \gamma_6^{(0)} \left[ \gamma_i^{(0)} \right] = 0$

indefinitely to produce coefficients for any other order Runge-Kutta process.

If in taking the product in the left member of equation (61) we use equations (32), we get, instead of equation (62), the matrix equation

$$\begin{bmatrix} c_3^{(1)} & c_3^{(2)} & c_3^{(3)} \\ \vdots & \vdots & \vdots \\ c_6^{(1)} & c_6^{(2)} & c_6^{(3)} \end{bmatrix} = \Omega_{2,6}^3 \begin{bmatrix} \frac{1}{2} \alpha_2^2 & \frac{1}{3} \alpha_3^3 & \frac{1}{4} \alpha_4^4 \\ \vdots & \vdots & \vdots \\ \frac{1}{2} \alpha_6^2 & \frac{1}{3} \alpha_6^3 & \frac{1}{4} \alpha_6^4 \end{bmatrix} \quad (64)$$

which is equation (35) with its right member unexpanded. If we expand the left member of equation (64), we see that terms like  $\omega_i c_i^{(n)} \alpha_i^j$  are also generalized Runge-Kutta weight coefficients. Evidently then, we can replace  $\omega_i$  in  $\gamma_i^{(n)} \omega_i$  by terms of this type also.<sup>12</sup>

If in equation (64) we replace  $\omega_i$  by  $\gamma_i^{(0)}$  in the terms  $\Omega_{2,6}^3$  and  $\Omega_{3,6}^3$  defined by equations (34), the right member can be evaluated by using equations (63). Thus, in the Runge-Kutta weights of the type  $\omega_i c_i^{(n)} \alpha_i^q$  we may replace the  $\omega_i$  by  $\gamma_i^{(0)}$ ; and by an extension of the preceding arguments  $\omega_i$  may also be replaced by  $\gamma_i^{(1)}$ ,  $\gamma_i^{(2)}$ , ..., etc., producing terms of the type  $\gamma_i^{(n)} c_i^{(m)} \alpha_i^q$ .

It should be recalled that equation (64) (or its general form for higher orders) is our basic matrix equation, which still gives valid Runge-Kutta equations with any generalized weights which may replace the elementary weights in  $\Omega_{2,6}^3$  and  $\Omega_{3,6}^3$ . We should keep this in mind below as we evaluate the matrix product  $\Omega C$  for the sixth order.

## THE SIXTH-ORDER RUNGE-KUTTA EQUATIONS

In Table I we have enumerated the generalized Runge-Kutta weight coefficients for the sixth-order process. We show only the first element of each row since the other elements in the row are simply obtained by advancing the subscripts to  $N$ . The  $\Omega$ -matrix can, of course, be easily expanded from the first four rows in Table I by the simple rules we have just given. It will be observed that if we limit ourselves to weight coefficients whose total degree is less than three we

<sup>12</sup> See, for instance,  $\gamma_3^{(0)} \left[ \omega_i c_i^{(1)} \right]$  in Table I.

will obtain the  $\Omega$ -matrix in equation (58) for the fifth order.<sup>13</sup> It is evident, then, that for any higher order Runge-Kutta process we need merely extend the list in Table I.

In the last four columns we give the numerical values corresponding to the matrix product  $\Omega C$  where these are pertinent;<sup>14</sup> and we shall next consider how these are evaluated.

## THE EVALUATION OF THE NUMERICAL MATRIX

The numerical values for the first four rows in Table I are given by equation (35); and we will illustrate how, by using previously derived results, we can determine the other numerical values shown in this table. For the sake of brevity we will limit ourselves only to those results just requisite to the sixth-order case with  $N$  evaluations. The extension to higher orders is amply evident.

From what has already been established, we can write the matrix equation, valid for  $n = 0, 1, 2$ :

$$\begin{aligned}
 & \begin{bmatrix} \gamma_3^{(n)} & \dots & \gamma_N^{(n)} \\ \gamma_3^{(n)} \alpha_3 & \dots & \gamma_N^{(n)} \alpha_N \\ \gamma_3^{(n)} \alpha_3^2 & \dots & \gamma_N^{(n)} \alpha_N^2 \end{bmatrix} \begin{bmatrix} c_3^{(1)} & c_3^{(2)} & c_3^{(3)} \\ c_4^{(1)} & c_4^{(2)} & c_4^{(3)} \\ \vdots & \vdots & \vdots \\ c_N^{(1)} & c_N^{(2)} & c_N^{(3)} \end{bmatrix} \\
 &= \begin{bmatrix} \gamma_2^{(n)} & \dots & \gamma_N^{(n)} \\ \gamma_2^{(n)} \alpha_2 & \dots & \gamma_N^{(n)} \alpha_N \\ \gamma_3^{(n)} \alpha_2^2 & \dots & \gamma_N^{(n)} \alpha_N^2 \end{bmatrix} \begin{bmatrix} \frac{1}{2} \alpha_2^2 & \frac{1}{3} \alpha_2^3 & \frac{1}{4} \alpha_2^4 \\ \vdots & \vdots & \vdots \\ \frac{1}{2} \alpha_N^2 & \frac{1}{3} \alpha_N^3 & \frac{1}{4} \alpha_N^4 \end{bmatrix} \\
 &= \begin{bmatrix} \frac{1}{2} \left[ \frac{1}{3} \frac{1}{(4+n)} \right] & \frac{1}{3} \left[ \frac{1}{4} \frac{1}{(5+n)} \right] & \frac{1}{4} \left[ \frac{1}{5} \frac{1}{(6+n)} \right] \\ \frac{1}{2} \left[ \frac{1}{4} \frac{1}{(5+n)} \right] & \frac{1}{3} \left[ \frac{1}{5} \frac{1}{(6+n)} \right] & \text{---} \\ \frac{1}{2} \left[ \frac{1}{5} \frac{1}{(6+n)} \right] & \text{---} & \text{---} \end{bmatrix} \quad (65)
 \end{aligned}$$

<sup>13</sup> For order  $p = m + 1$ , the weight coefficients must include those of total degree  $m - 2$ .

<sup>14</sup>  $C$  is a  $(N \times 4)$  matrix. Butcher [4] gives a construction for the sixth order with  $N = 7$ ; H  ta [3] originally gave one with  $N = 8$ .

where we have evaluated the right side by using equation (62) or (63). These, and subsequent results, have been used in the appropriate place in Table I.

$$\begin{aligned}
 & \text{Again, starting with the basic equation} \\
 & \begin{bmatrix} \gamma_3^{(0)} \left( \gamma_i^{(0)} \right) & \dots & \gamma_N^{(0)} \left( \gamma_i^{(0)} \right) \\ \gamma_3^{(0)} \left( \gamma_i^{(0)} \right) \alpha_3 & \dots & \gamma_N^{(0)} \left( \gamma_i^{(0)} \right) \alpha_N \end{bmatrix} \begin{bmatrix} c_3^{(1)} & c_3^{(2)} \\ \vdots & \vdots \\ c_N^{(1)} & c_N^{(2)} \end{bmatrix} \\
 &= \begin{bmatrix} \gamma_2^{(0)} \left( \gamma_i^{(0)} \right) & \dots & \gamma_N^{(0)} \left( \gamma_i^{(0)} \right) \\ \gamma_2^{(0)} \left( \gamma_i^{(0)} \right) \alpha_2 & \dots & \gamma_N^{(0)} \left( \gamma_i^{(0)} \right) \alpha_N \end{bmatrix} \begin{bmatrix} \frac{1}{2} \alpha_2^2 & \frac{1}{3} \alpha_2^3 \\ \vdots & \vdots \\ \frac{1}{2} \alpha_N^2 & \frac{1}{3} \alpha_N^3 \end{bmatrix} \\
 &= \begin{bmatrix} \frac{1}{2} \left( \frac{1}{3} \frac{1}{4} \frac{1}{5} \right) & \frac{1}{3} \left( \frac{1}{4} \frac{1}{5} \frac{1}{6} \right) \\ \frac{1}{2} \left( \frac{1}{4} \frac{1}{5} \frac{1}{6} \right) & \text{---} \end{bmatrix} \quad (66)
 \end{aligned}$$

we again get the numerical results by using equation (63).

Similarly, we can write

$$\begin{aligned}
 & \begin{bmatrix} \gamma_3^{(0)} \left( \gamma_i^{(1)} \right) & \dots & \gamma_N^{(0)} \left( \gamma_i^{(1)} \right) \end{bmatrix} \begin{bmatrix} c_3^{(1)} \\ \vdots \\ c_N^{(1)} \end{bmatrix} \\
 &= \begin{bmatrix} \gamma_2^{(0)} \left( \gamma_i^{(1)} \right) & \dots & \gamma_N^{(0)} \left( \gamma_i^{(1)} \right) \end{bmatrix} \begin{bmatrix} \frac{1}{2} \alpha_2^2 \\ \vdots \\ \frac{1}{2} \alpha_N^2 \end{bmatrix} \quad (67)
 \end{aligned}$$

and if we replace  $\omega_i$  by  $\gamma_i^{(1)}$  in equation (61), and use equation (59), we get

$$\begin{bmatrix} \gamma_2^{(0)} \left( \gamma_i^{(1)} \right) & \dots & \gamma_{N-1}^{(0)} \left( \gamma_i^{(1)} \right) \end{bmatrix} \begin{bmatrix} \alpha_2 & \alpha_2^2 \\ \vdots & \vdots \\ \alpha_{N-1} & \alpha_{N-1}^2 \end{bmatrix}$$

TABLE I. THE GENERALIZED RUNGE-KUTTA WEIGHT COEFFICIENTS FOR THE SIXTH ORDER

First Coefficient *	Total Degree								
$\omega_3$	0	$\frac{1}{2}$	$\frac{1}{3}$			$\frac{1}{3}$	$\frac{1}{4}$		$\frac{1}{4}$
$\omega_3 \alpha_3$	1	$\frac{1}{2}$	$\frac{1}{4}$			$\frac{1}{3}$	$\frac{1}{5}$		$\frac{1}{4}$
$\omega_3 \alpha_3^2$	2	$\frac{1}{2}$	$\frac{1}{5}$			$\frac{1}{3}$	$\frac{1}{6}$		-
$\omega_3 \alpha_3^3$	3	$\frac{1}{2}$	$\frac{1}{6}$			-	-		-
$\gamma_3^{(0)}$	1	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{4}$		$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{5}$	-
$\gamma_3^{(0)} \alpha_3$	2	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{5}$		$\frac{1}{3}$	$\frac{1}{5}$	$\frac{1}{6}$	-
$\gamma_3^{(0)} \alpha_3^2$	3	$\frac{1}{2}$	$\frac{1}{5}$	$\frac{1}{6}$		-	-	-	-
$\gamma_3^{(1)}$	2	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{5}$		$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{6}$	-
$\gamma_3^{(1)} \alpha_3$	3	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{6}$		-	-	-	-
$\gamma_3^{(2)}$	3	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{6}$		-	-	-	-
$\gamma_3^{(0)} \left( \gamma_i^{(0)} \right)$	2	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{5}$	$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{5}$	$\frac{1}{6}$
$\gamma_3^{(0)} \left( \gamma_i^{(0)} \right) \alpha_3$	3	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{5}$	$\frac{1}{6}$	-	-	-	-
$\gamma_3^{(0)} \left( \gamma_i^{(1)} \right)$	3	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{6}$	-	-	-	-
$\gamma_3^{(1)} \left( \gamma_i^{(0)} \right)$	3	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{5}$	$\frac{1}{6}$	-	-	-	-
$\gamma_3^{(0)} \left[ \gamma_i^{(0)} \left( \gamma_j^{(0)} \right) \right]$	3	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{5}$	$\frac{1}{6}$	-	-	-
$\gamma_3^{(0)} \left( \omega_i c_i^{(1)} \right)$	3	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{2}$	$\frac{1}{6}$	-	-	-	-
$\omega_3 c_3^{(1)}$	2	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{5}$		$\frac{1}{3}$	$\frac{1}{2}$	$\frac{1}{6}$	-
$\omega_3 c_3^{(1)} \alpha_3$	3	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{6}$		-	-	-	-
$\omega_3 c_3^{(2)}$	3	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{6}$		-	-	-	-
$\gamma_3^{(0)} c_3^{(1)}$	3	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{5}$	$\frac{1}{6}$	-	-	-	-

\* Only the first weight coefficient (element) of each row of the  $\Omega$ -matrix is shown; the other elements in the row are simply obtained by advancing the subscripts to N. In the last four columns are given the values of  $\Omega C$ .

\*\* These two are easily seen to be repetitions of each other.



$$\begin{aligned}
&= \begin{bmatrix} \gamma_2^{(1)} & \gamma_3^{(1)} & \dots & \gamma_N^{(1)} \end{bmatrix} \begin{bmatrix} \frac{1}{2} \alpha_2^2 & \frac{1}{3} \alpha_2^3 \\ \vdots & \vdots \\ \frac{1}{2} \alpha_N^2 & \frac{1}{3} \alpha_N^3 \end{bmatrix} \quad (68) \quad \begin{bmatrix} \gamma_3^{(0)} \left( \gamma_i^{(1)} \right) & \dots & \gamma_N^{(0)} \left( \gamma_i^{(1)} \right) \end{bmatrix} \begin{bmatrix} c_3^{(1)} \\ c_4^{(1)} \\ \vdots \\ c_N^{(1)} \end{bmatrix} \\
&= \begin{bmatrix} \frac{1}{2} \begin{bmatrix} \frac{1}{3} & \frac{1}{5} \end{bmatrix} & \frac{1}{3} \begin{bmatrix} \frac{1}{4} & \frac{1}{6} \end{bmatrix} \end{bmatrix} = \frac{1}{2} \begin{bmatrix} \frac{1}{3} & \left( \frac{1}{4} \quad \frac{1}{6} \right) \end{bmatrix}. \quad (69)
\end{aligned}$$

where the last evaluation was made by using equation (62); so that, combining the results in equations (67) and (68), we get

#### REFERENCES

1. Kopal, Z.: Numerical Analysis. John Wiley & Sons, New York, 1955, p. 196.
2. Butcher, J. C.: Coefficients for the Study of Runge-Kutta Integration Processes. J. Austral. Math. Soc., vol. 3, 1963, pp. 185-201.
3. Butcher, J. C.: On the Integration Process of A. H<sup>A</sup>ta. J. Austral. Math. Soc., vol. 3, 1963, pp. 202-206.
4. Butcher, J. C.: On Runge-Kutta Processes of High Order. J. Austral. Math. Soc., vol. 4, 1964, pp. 179-194.
5. Butcher, J. C.: On the Attainable Order of Runge-Kutta Methods. Math. Comput., vol. 19, no. 91, July, 1965, pp. 408-17.
6. Shanks, E. B.: Higher Order Approximations of Runge-Kutta Type. NASA TN D-2920, Sept. 1965, p. 6.
7. Shanks, E. B.: Solutions of Differential Equations by Evaluations of Functions. Math. of Comp. vol. 20, no. 93, January, 1966.
8. Lanczos, C.: Applied Analysis. Prentice-Hall, Englewood Cliff, N. J., 1956, p. 274.
9. Hildebrand, F. B.: Introduction to Numerical Analysis. McGraw-Hill, New York, 1956, p. 351.
10. Luther, H. A.; and Konen, H. P.: Some Fifth-Order Classical Runge-Kutta Formulas. SIAM Rev. vol. 7, no. 4, Oct. 1965, pp. 551-558.

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